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# TWISTAROMA

Caractérisation et dosage des arômes et antioxydants  
Expertises, R&D

## ESSAI R&D TWISTAROMA

**Sample :** Café capsule

**Analytical method :** SBSE

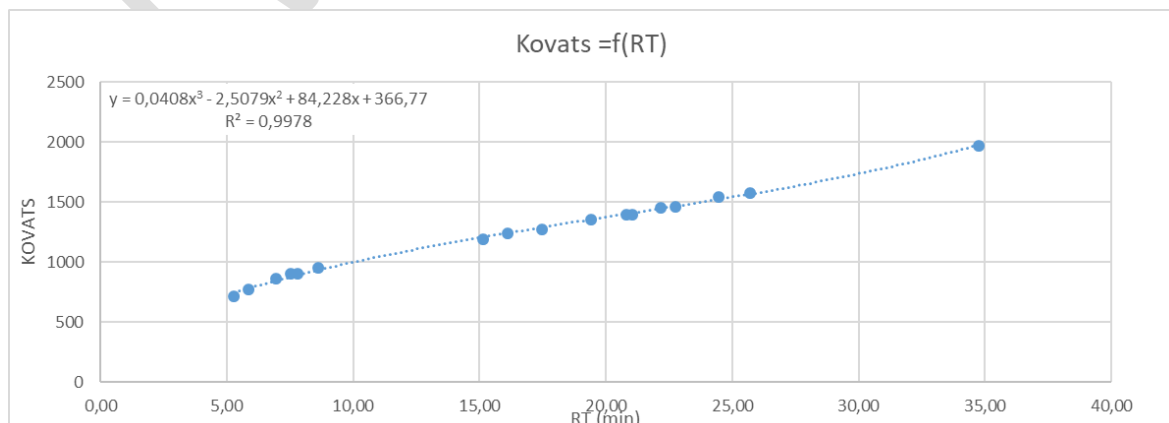
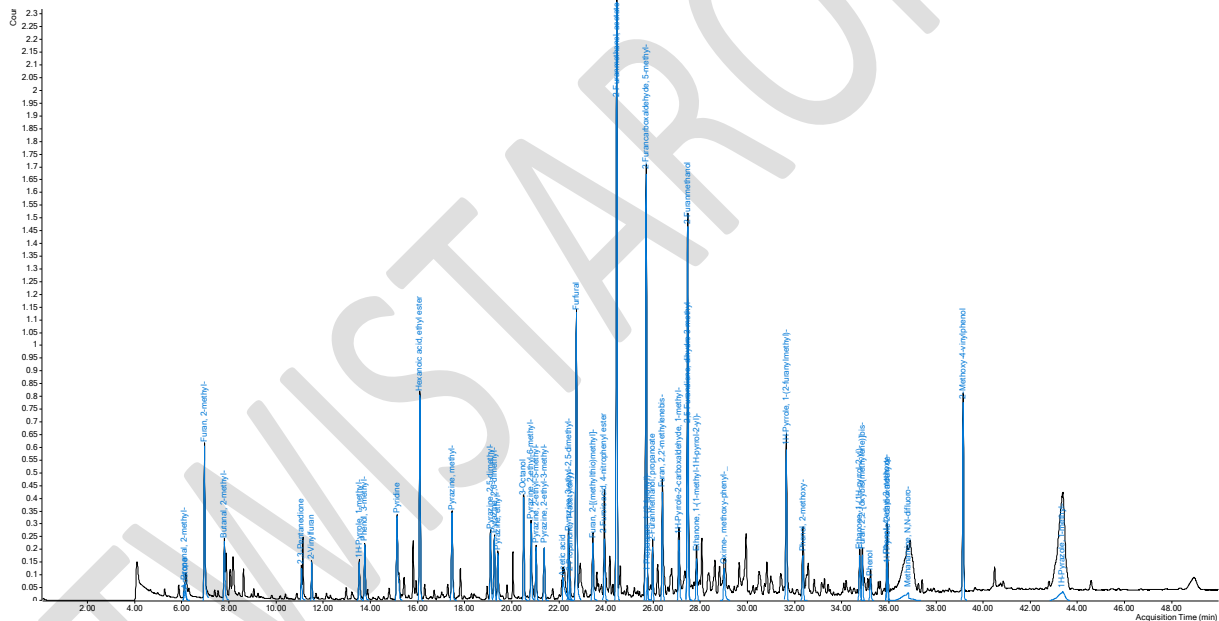
**Carrier gas :** Helium

**GC :** Agilent 7890

**MS :** Agilent 5977B inert MSD

**Column :** DB-Wax capillary column

**Identification :** Déconvolution, NIST14 et RI





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CAS	nom_officiel	RT (min)	Descriptions (main)	Concentration (µg/L eq 3-octanol)
78-79-5	Isoprene (2-Methyl-1,3-Butadiene)	4,67		1,19
74-93-1	Methanethiol	4,85	sulfury	0,57
75-15-0	Carbon disulfide	5,27	unpleasant, loud	18,65
75-18-3	Dimethyl sulfide	5,42	sulfury, cabbage, Truffle	0,78
503-30-0	Oxetane	5,82	pleasant, aromatic	2,75
110-00-9	Furan	5,87	unknown,	18,22
78-84-2	isobutanal	6,14	malty, green	37,61
67-64-1	2-Propanone	6,14	unknown	30,35
79-20-9	Methyl acetate	6,30	fruit,	11,47
534-22-5	2-methylfuran	6,96	unknown,	160,80
123-72-8	1-butanal	7,08	pungent	0,97
141-78-6	Ethyl acetate	7,23	fruit, pine apple, sweet	1,26
930-27-8	3-methyl furan	7,40		5,97
78-93-3	2-Butanone	7,54	acetone, etheric	12,98
554-12-1	Methyl propanoate	7,62	rum, strawberry, apple	0,71
96-17-3	2-methyl butanal	7,81	malty, green	57,29
590-86-3	3-methyl butanal	7,88	malty, chocolate, green	27,85
625-86-5	2,5-Dimethylfuran	8,62		22,97
431-03-8	Diacetyl	9,06	butter, pastry	20,90
107-87-9	2-Pentanone	9,22	fruit, thinner	3,00
3299-32-9	2,4,5-trimethyl-1,3-dioxolane	9,32		0,55
3208-16-0	2-Ethylfuran	9,38	rubber, sweet	1,43
556-24-1	Methyl isopentanoate	10,18		1,25
110-02-1	Thiophene	10,39	sulfury	5,21
1703-52-2	2-Ethyl-5-methylfuran	10,49	burned, fresh	1,85
1191-99-7	2,3-DIHYDROFURAN	10,86		2,69
108-88-3	Toluene	10,89	sweet, synthetic	6,04
1192-62-7	1-(2-furanyl)-Ethanone	11,00	sweet	0,50
600-14-6	2,3-pentanedione	11,07	creamy, pungent	44,30
108-64-5	Ethyl isopentanoate	11,37	sweet	0,18
1487-18-9	2-Vinylfuran	11,51		39,20
624-92-0	Dimethyl disulfide	11,69	onion, cabbage, Truffle	4,49
66-25-1	Hexanal	11,77	green, grassy, fruit	0,70
554-14-3	2-methylthiophene	12,14	sulfury,	9,20
1115-11-3	2-methyl-2-butenal	12,30		4,40
123-92-2	Isoamyl acetate	12,83	banana, fruit, sweet	1,64
616-44-4	3-methylthiophene	12,94		2,25



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3848-24-6	Hexan-2,3-dione	12,97		19,69
100-41-4	Ethyl benzene	13,13		1,44
539-82-2	Ethyl pentanoate	13,20	fruit, apple, floral	0,39
4437-51-8	Hexan-3,4-dione	13,22	butter, toasted, almond, caramel	15,87
625-33-2	Pent-3-en-2-one	13,27	acetone, fish, fruity	4,62
96-54-8	1-Methyl-1H-pyrrole	13,53	strong, smoky, wood, herbal	44,38
108-38-3	1,3-dimethylbenzene	13,56	plastic,	1,64
96-04-8	Heptan-2,3-dione	13,58		3,47
123-35-3	b-myrcene	13,88	spicy	6,71
924-50-5	Methyl 3-methyl-2-butenolate	14,36		0,94
110-43-0	2-Heptanone	14,75	fruit, bluecheese, sweet	1,88
617-92-5	Ethyl-pyrrole	14,79	unknown,	7,52
5205-07-2	3-Methyl-3-buten-1-ol, acetate	15,00		0,56
110-86-1	Pyridine	15,13	burnt,	147,57
5989-27-5	d-Limonene	15,21	grassy,	2,30
54750-69-5	cis-anhydro linalool oxide	15,53		0,77
625-84-3	2,5-Dimethylpyrrole	15,62		3,80
632-15-5	3,4-Dimethylthiophene	15,74		0,25
290-37-9	Pyrazine	15,85	coffee,	12,28
3777-69-3	2-Pentylfuran	16,01	fruit, sweet	2,23
109-06-8	2-methylpyridine	16,17	sweet	2,17
123-66-0	Ethyl hexanoate	16,20	fruit, green apple, sweet	125,51
13679-46-4	Furfuryl methyl ether	16,30	Herbal,	12,68
1191-16-8	3-methyl-2-butenyl acetate	16,71		5,30
106-68-3	3-Octanone	16,84	fruit, sweet	0,54
100-42-5	Styrene	17,03	sweet	7,51
3188-00-9	2-methyltetrahydrofuran-3-one	17,28	nutty	19,69
527-84-4	o-Cymene	17,38		0,72
109-08-0	2-methylpyrazine	17,46	green, toasted	134,08
526-73-8	Hemimellitene	17,80	metallic, mouldy, dirty	0,67
541-58-2	2,4-Dimethylthiazole	17,97		0,91
116-09-6	Acetol	18,39	unknown, nutty,	9,63
108-99-6	Pyridine, 3-methyl-	18,41		2,76
543-49-7	2-Heptanol	18,46	fruit, earthy, sweet	2,73
106-30-9	Ethyl heptanoate	18,95	fruit, wine	7,04
123-32-0	2,5(6)-dimethylpyrazine	19,10	roasted, toasted	92,71
108-50-9	2,6-dimethylpyrazine	19,26	roasted, roasted nut	87,68



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13925-00-3	2-ethyl pyrazine	19,41	roasted, wood	59,26
5910-89-4	2,3 Dimethyl Pyrazine	19,80	nutty, toasted	14,44
589-98-0	3-Octanol	20,51	mushroom, melon, citrus, mint	75,00
13925-03-6	2-ethyl-6-methylpyrazine	20,82	toasted	101,51
536-78-7	3-ethylpyridine	20,89	tobacco, leather	9,08
3658-80-8	dimethyl trisulfide	20,90	sulfury, cabbage, onion	2,09
13360-64-0	2-Ethyl 3- and 5-methylpyrazine	21,03	roasted, toasted	63,76
19961-52-5	5-Ethyl-2-methylthiazole	21,31		1,07
15707-23-0	2-Ethyl 3-methylpyrazine	21,37	roasted, potato	80,91
18138-03-9	2-(n-propyl)-Pyrazine	21,74	Herbal,	10,10
13067-27-1	2,6-diethylpyrazine	22,13	toasted,	21,94
64-19-7	Acetic acid	22,16	vinegar	50,97
4177-16-6	2-ethenylpyrazine	22,22	branch, nuts, burnt	12,88
13360-65-1	2,5-dimethyl 3-ethylpyrazine	22,41	potato, roasted	64,23
98-01-1	Furfural	22,41	alkane, sweet, floral	363,65
592-20-1	2-Oxopropyl acetate	22,46	unpleasant,	59,54
930-68-7	1-cyclohexen-3-one	22,52	roasted, savory, green	1,66
34995-77-2	trans-linalool oxide furanoid	22,62	floral, wood	8,10
15707-24-1	2,3,Diethylpyrazine	22,65	nuts, pepper	1,92
104-76-7	2-Ethyl hexanol	23,10	green, floral, rose	2,77
1438-91-1	2-Furfuryl methylsulfide	23,44	coffee,	84,01
13925-09-2	2-ethenyl-6-methylpyrazine	23,61	roasted, smoky	20,04
18138-05-1	3,5-Diethyl-2-methylpyrazine	23,68	sweet, vegetable	15,86
13925-08-1	2-ethenyl-5-methylpyrazine	23,81	coffee	13,26
109-97-7	1H-pyrrole	24,01	sweet,	18,32
271-89-6	2,3-Benzofuran (Cumaron)	24,07		9,78
50746-10-6	3-Mercapto-3-methylbutyl formate	24,24		2,30
1575-57-1	1-(acetyloxy)-2-Butanone	24,29		14,65
123-29-5	Ethyl nonanoate	24,39	fruit, rose, floral	7,67
24683-00-9	2-Isobutyl-3-methoxypyrazine	24,40	earthy, bean, spicy	5,54
623-17-6	2-Furfuryl acetate	24,46	nutty,	476,82

La reproduction de ce rapport n'est autorisée que sous sa forme intégrale et est soumise à l'autorisation du laboratoire.

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100-52-7	Benzaldehyde	24,60	almond, nutty, wood	24,56
79-09-4	Propanoic acid	24,67	pungent, rancid, soy	3,13
13679-85-1	2-methyl dihydro3-(2H)-thiophenone	24,78	wet,	5,55
1193-79-9	2-acetyl-5-methylfuran	25,21	nutty, strong	58,21
620-02-0	5-methylfurfural	25,70	caramel, spicy	485,48
3194-15-8	1-(2-Furyl)propan-1-one	25,75		51,24
7295-76-3	3-Methoxy-pyridine	26,09		0,71
1197-40-6	2-Furfurylfuran	26,39	earthy,	88,81
1122-62-9	2-Acetylpyridine	26,63	roasted,	6,11
4265-25-2	2-methyl benzofuran	26,66		1,26
5905-00-0	2,2-Bifuran	26,75		41,49
1192-58-1	1-methylpyrroltrans-2-carbaldehyde	27,02	butter,	65,94
109-52-4	Pentanoic acid	27,03	sweaty, sweat	1,58
98-00-0	2-Furanmethanol	27,47	burnt, sweet	234,78
122-78-1	2-phenylacetaldehyde	27,51	floral, honey, rose	32,27
932-16-1	2-Acetyl-1-methylpyrrole	27,85		47,84
503-74-2	3-methyl butanoic acid	27,91	rancid, cheesy, acidic	17,68
98-03-3	Thiophene-2-carbaldehyde	28,81	vinous, unknown	14,41
22047-26-3	2-Acetyl-6-methylpyrazine	28,83	grilled coffee, cocoa, popcorn	9,18
13679-70-4	5-methyl-2-thiophenecarbaldehyde	29,98	meaty,	9,11
101-41-7	Methyl benzene Acetate	30,16	sweet, unknown	1,98
88-15-3	2-acetylthiophene	30,72	odor,	12,74
122-00-9	4-methylacetophenone	30,78	fruit, sweet	3,37
119-36-8	Methyl salicylate	30,83	sweet, minty, spicy	12,53
1438-94-4	furfuryl pyrrole	31,65	roasted, green	186,84
23726-93-4	trans-b-Damascenone	31,71	apple, honey	8,50
13679-41-9	3-phenylfuran	32,34	green, nutty	10,44
90-05-1	Guaiacol	32,35	burnt, smoky	43,21
6846-50-0	[2 4,4-trimethyl-1-(2-methylpropanoyloxy)pentan-3-yl]2-methylpropanoate	32,94	moldy	0,65
21835-01-8	3-Ethylcyclopentan-1,2-dione	33,14		6,27
589-18-4	4-methylbenzyl alcohol	33,25	floral	0,82
60-12-8	2-Phenylethanol	33,50	rose, floral, honey	5,43
1072-83-9	2-Acetylpyrrole	34,76	walnut	49,25
4437-22-3	difurfuryl ether	34,88	unpleasant,	55,17
118-71-8	Maltol	34,95	caramel, burnt sugar,	28,69



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108-95-2	Phenol	35,22	medicinal, smoky	30,20
6380-23-0	1,2-Dimethoxy-4-vinylbenzene	35,81		5,20
3658-77-3	Furaneol	35,86	caramel, sweet, burnt	2,32
2785-89-9	4-Ethyl guaiacol	35,92	spicy, clove, smoky	53,36
1003-29-8	2-Formylpyrrole	35,93	unpleasant	43,75
106-44-5	p-Cresol	36,02	phenolic, cattle, medicinal	15,31
122-99-6	2-phenoxyethanol	38,18	unknown,	1,52
123-07-9	4-Ethyl phenol	38,56	phenolic, leather, stable	5,47
112-05-0	Nonanoic acid	38,68	fatty, rancid	0,80
7786-61-0	4-vinyl guaiacol	39,15	spicy, clove, smoky	169,29

Illkirch, le 1er avril 2019

Dr. Damien Steyer  
Directeur du laboratoire